



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:34 PM UTC

PDB ID : 1GO6 / pdb_00001go6
Title : Balhimycin in complex with Lys-D-ala-D-ala
Authors : Lehmann, C.; Bunkoczi, G.; Vertesy, L.; Sheldrick, G.M.
Deposited on : 2001-10-19
Resolution : 0.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

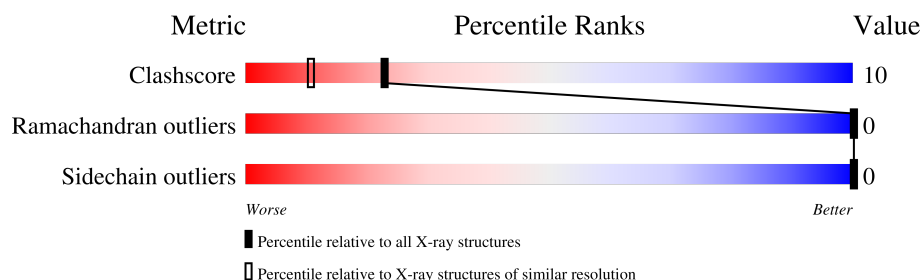
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 0.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1197 (1.02-0.94)
Ramachandran outliers	187476	1136 (1.02-0.94)
Sidechain outliers	187428	1137 (1.02-0.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	7	29% 57% 14%
1	C	7	14% 57% 29%
1	E	7	14% 86%
1	G	7	14% 71% 14%
1	I	7	14% 57% 29%
1	K	7	14% 71% 14%
1	M	7	14% 71% 14%
1	O	7	29% 57% 14%

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Mol	Chain	Length	Quality of chain
2	B	3	 67%33%
2	D	3	 100%
2	F	3	 100%
2	H	3	 67%33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CIT	I	20	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 1340 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

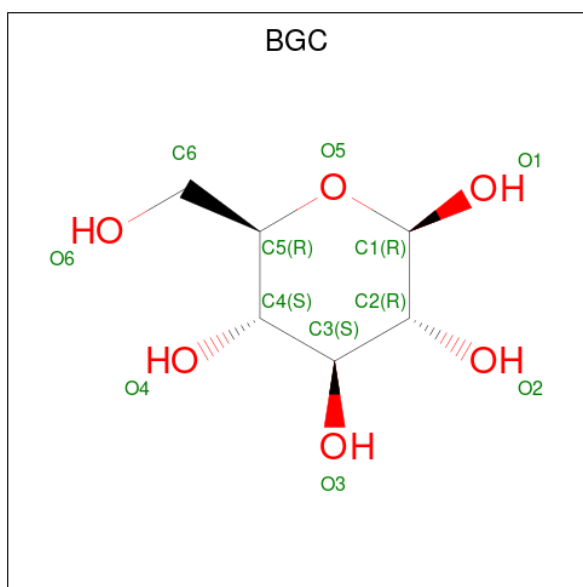
- Molecule 1 is a protein called BALHIMYCIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	7	Total	C	Cl	N	O	0	0	0
			80	53	2	8	17			
1	C	7	Total	C	Cl	N	O	0	0	0
			80	53	2	8	17			
1	E	7	Total	C	Cl	N	O	0	1	0
			83	55	2	9	17			
1	G	7	Total	C	Cl	N	O	0	1	0
			82	54	2	8	18			
1	I	7	Total	C	Cl	N	O	0	2	0
			91	61	2	10	18			
1	K	7	Total	C	Cl	N	O	0	2	0
			91	61	2	10	18			
1	M	7	Total	C	Cl	N	O	0	2	0
			83	54	2	8	19			
1	O	7	Total	C	Cl	N	O	0	3	0
			93	62	2	10	19			

- Molecule 2 is a protein called PEPTIDE LYS-DAL-DAL.

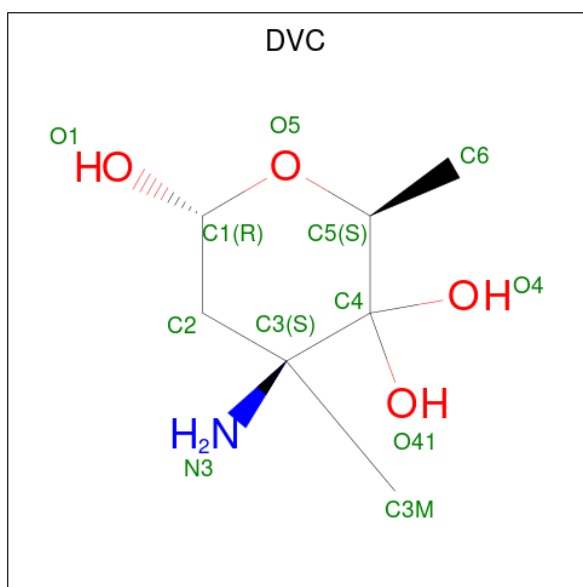
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	1	0
			27	17	6	4			
2	D	3	Total	C	N	O	0	1	0
			27	17	6	4			
2	F	3	Total	C	N	O	0	2	0
			31	19	7	5			
2	H	3	Total	C	N	O	0	0	0
			20	12	4	4			

- Molecule 3 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



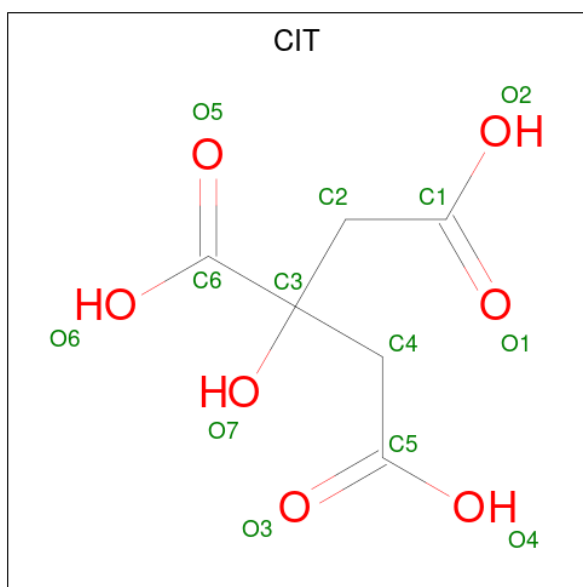
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	E	1	Total	C	O	0	0
			11	6	5		
3	G	1	Total	C	O	0	0
			11	6	5		
3	I	1	Total	C	O	0	0
			11	6	5		
3	K	1	Total	C	O	0	0
			11	6	5		
3	M	1	Total	C	O	0	1
			22	12	10		
3	O	1	Total	C	O	0	1
			14	8	6		

- Molecule 4 is (2R,4S,6S)-4-azanyl-4,6-dimethyl-oxane-2,5,5-triol (CCD ID: DVC) (formula: $C_7H_{15}NO_4$).



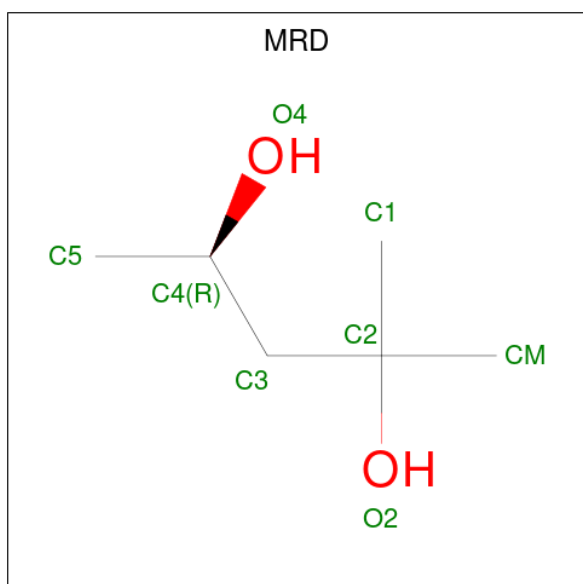
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			11	7	1	3		
4	C	1	Total	C	N	O	0	0
			11	7	1	3		
4	E	1	Total	C	N	O	0	0
			11	7	1	3		
4	G	1	Total	C	N	O	0	1
			22	14	2	6		
4	I	1	Total	C	N	O	0	0
			11	7	1	3		
4	K	1	Total	C	N	O	0	0
			11	7	1	3		
4	M	1	Total	C	N	O	0	1
			22	14	2	6		
4	O	1	Total	C	N	O	0	1
			22	14	2	6		

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



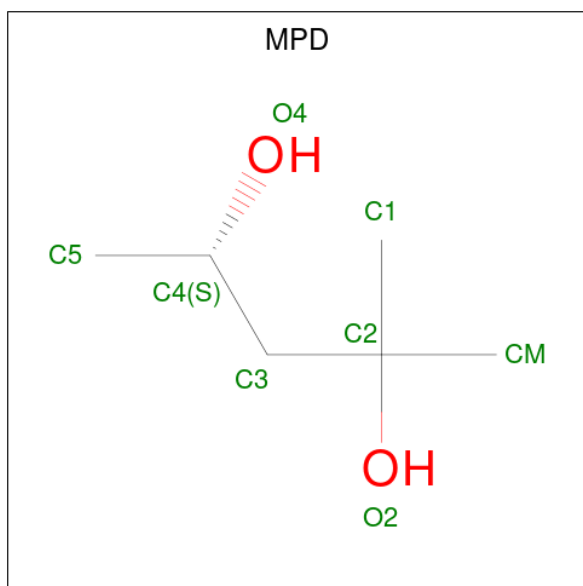
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			9	4	5		
5	I	1	Total	C	O	0	0
			13	6	7		
5	K	1	Total	C	O	0	0
			6	3	3		
5	M	1	Total	C	O	0	0
			13	6	7		
5	O	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	I	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	K	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	27	Total	O	0	0
			27	27		
8	B	10	Total	O	0	0
			10	10		
8	C	22	Total	O	0	0
			22	22		
8	D	7	Total	O	0	0
			7	7		
8	E	25	Total	O	0	0
			25	25		
8	F	8	Total	O	0	0
			8	8		
8	G	26	Total	O	0	0
			26	26		
8	H	6	Total	O	0	0
			6	6		

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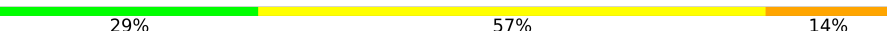
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	27	Total 27	O 27	0	0
8	K	31	Total 31	O 31	0	0
8	M	32	Total 32	O 32	0	0
8	O	38	Total 38	O 38	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

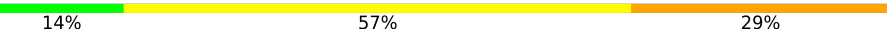
Note EDS was not executed.

• Molecule 1: BALHIMYCIN

Chain A: 



• Molecule 1: BALHIMYCIN

Chain C: 

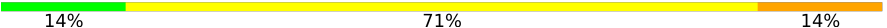


• Molecule 1: BALHIMYCIN

Chain E: 

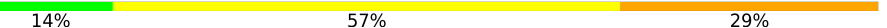


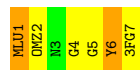
• Molecule 1: BALHIMYCIN

Chain G: 

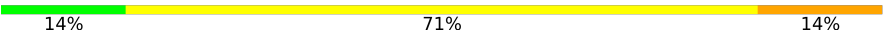


• Molecule 1: BALHIMYCIN

Chain I: 

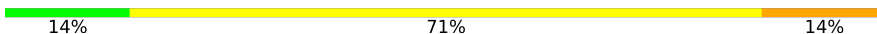


• Molecule 1: BALHIMYCIN

Chain K: 

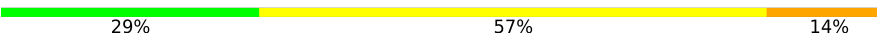


- Molecule 1: BALHIMYCIN

Chain M:  14% 71% 14%



- Molecule 1: BALHIMYCIN

Chain O:  29% 57% 14%

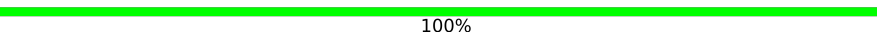


- Molecule 2: PEPTIDE LYS-DAL-DAL

Chain B:  67% 33%

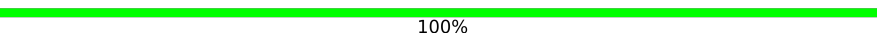


- Molecule 2: PEPTIDE LYS-DAL-DAL

Chain D:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: PEPTIDE LYS-DAL-DAL

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: PEPTIDE LYS-DAL-DAL

Chain H:  67% 33%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.93Å 28.02Å 50.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.00 – 0.98	Depositor
% Data completeness (in resolution range)	98.6 (89.00-0.98)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.130 , 0.159	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1340	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, 3FG, MPD, OMZ, OMY, CIT, GHP, BGC, DAL, DVC, MLU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.71	0/7	0.73	0/8
1	C	0.57	0/7	0.79	0/8
1	E	0.65	0/7	0.78	0/8
1	G	1.28	0/7	1.14	0/8
1	I	0.84	0/7	2.02	0/8
1	K	1.21	0/7	1.18	0/8
1	M	1.38	0/7	1.69	0/8
1	O	0.67	0/7	1.29	0/8
2	B	0.44	0/16	0.60	0/16
2	D	0.68	0/16	0.94	0/16
2	F	0.38	0/16	0.94	0/16
2	H	1.03	0/8	3.21	1/8 (12.5%)
All	All	0.81	0/112	1.36	1/120 (0.8%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	LYS	CG-CD-CE	6.97	127.34	111.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	80	0	45	1	0
1	C	80	0	43	2	0
1	E	83	0	43	2	0
1	G	82	0	42	2	0
1	I	91	0	59	3	0
1	K	91	0	58	1	0
1	M	83	0	40	1	0
1	O	93	0	59	1	0
2	B	27	0	38	3	0
2	D	27	0	38	0	0
2	F	31	0	42	0	0
2	H	20	0	23	1	0
3	A	11	0	10	0	0
3	C	11	0	9	0	0
3	E	11	0	10	0	0
3	G	11	0	9	0	0
3	I	11	0	9	0	0
3	K	11	0	10	0	0
3	M	22	0	18	0	0
3	O	14	0	9	0	0
4	A	11	0	13	0	0
4	C	11	0	13	0	0
4	E	11	0	13	1	0
4	G	22	0	26	4	0
4	I	11	0	13	0	0
4	K	11	0	13	0	0
4	M	22	0	26	0	0
4	O	22	0	26	1	0
5	E	9	0	3	3	0
5	I	13	0	5	2	0
5	K	6	0	3	1	0
5	M	13	0	5	0	0
5	O	13	0	5	0	0
6	I	8	0	14	0	0
7	K	8	0	14	0	0
8	A	27	0	0	1	0
8	B	10	0	0	2	0
8	C	22	0	0	1	0
8	D	7	0	0	1	0
8	E	25	0	0	0	0
8	F	8	0	0	0	0
8	G	26	0	0	2	0
8	H	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	27	0	0	0	0
8	K	31	0	0	0	0
8	M	32	0	0	1	0
8	O	38	0	0	1	0
All	All	1340	0	806	20	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:9[A]:DVC:O4	8:O:2036:HOH:O	1.63	1.16
5:E:20:CIT:C3	4:G:9[B]:DVC:HN3A	1.92	0.83
8:G:2015:HOH:O	2:H:1:LYS:HG3	1.84	0.77
1:E:3:ASN:OD1	5:E:20:CIT:H21	1.88	0.72
1:A:2:OMZ:CL	8:A:2023:HOH:O	2.44	0.72
1:C:1:MLU:O	5:E:20:CIT:H22	1.91	0.71
1:I:6:OMY:CL	5:I:20:CIT:H41	2.31	0.68
4:G:9[B]:DVC:H6	8:G:2016:HOH:O	2.03	0.58
2:B:1[A]:LYS:HG2	8:D:2007:HOH:O	2.06	0.55
1:C:2:OMZ:CL	8:C:2016:HOH:O	2.56	0.54
1:I:1[A]:MLU:O	1:I:1[A]:MLU:HCN2	2.13	0.49
1:M:1:MLU:HD23	8:M:2032:HOH:O	2.13	0.48
1:G:6[A]:OMY:ODE	4:G:9[A]:DVC:H3MA	2.13	0.48
1:I:1[A]:MLU:HA	5:I:20:CIT:O2	2.14	0.47
1:O:1[B]:MLU:HD22	1:O:3:ASN:ND2	2.29	0.47
2:B:1[A]:LYS:HA	8:B:2010:HOH:O	2.14	0.46
1:K:1[A]:MLU:HA	5:K:20:CIT:O2	2.16	0.46
1:E:3:ASN:HA	4:G:9[B]:DVC:H3MB	1.98	0.45
2:B:1[B]:LYS:NZ	8:B:2003:HOH:O	2.50	0.44
4:E:9:DVC:H3MB	1:G:3:ASN:HA	2.01	0.42

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1/7 (14%)	1 (100%)	0	0	100	100
1	C	1/7 (14%)	1 (100%)	0	0	100	100
1	E	1/7 (14%)	1 (100%)	0	0	100	100
1	G	1/7 (14%)	0	1 (100%)	0	100	100
1	I	1/7 (14%)	1 (100%)	0	0	100	100
1	K	1/7 (14%)	1 (100%)	0	0	100	100
1	M	1/7 (14%)	1 (100%)	0	0	100	100
1	O	1/7 (14%)	0	1 (100%)	0	100	100
All	All	8/56 (14%)	6 (75%)	2 (25%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1/1 (100%)	1 (100%)	0	100	100
1	C	1/1 (100%)	1 (100%)	0	100	100
1	E	1/1 (100%)	1 (100%)	0	100	100
1	G	1/1 (100%)	1 (100%)	0	100	100
1	I	1/1 (100%)	1 (100%)	0	100	100
1	K	1/1 (100%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	1/1 (100%)	1 (100%)	0	100	100
1	O	1/1 (100%)	1 (100%)	0	100	100
2	B	2/1 (200%)	2 (100%)	0	100	100
2	D	2/1 (200%)	2 (100%)	0	100	100
2	F	2/1 (200%)	2 (100%)	0	100	100
2	H	1/1 (100%)	1 (100%)	0	100	100
All	All	15/12 (125%)	15 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	3	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

68 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	MLU	K	1[B]	1	7,8,9	1.08	1 (14%)	7,9,11	1.76	3 (42%)
1	MLU	O	1[A]	1	7,8,9	1.93	3 (42%)	7,9,11	1.61	1 (14%)
1	GHP	I	4	1,3	10,11,12	1.48	3 (30%)	11,14,16	1.16	1 (9%)
1	3FG	G	7	1	12,13,13	0.68	0	14,18,18	0.92	1 (7%)
1	GHP	E	5	1	10,11,12	0.97	0	11,14,16	1.37	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLU	I	1[A]	1	7,8,9	0.91	0	7,9,11	1.58	1 (14%)
1	OMY	E	6	1,4	12,14,15	0.96	0	17,19,21	1.29	2 (11%)
1	OMZ	E	2	1	12,14,15	0.94	1 (8%)	17,19,21	1.27	2 (11%)
1	GHP	C	4	1,3	10,11,12	1.55	3 (30%)	11,14,16	1.36	2 (18%)
1	GHP	I	5	1	10,11,12	0.94	1 (10%)	11,14,16	1.14	1 (9%)
1	3FG	K	7	1	12,13,13	1.19	1 (8%)	14,18,18	1.48	3 (21%)
1	3FG	A	7	1	12,13,13	1.05	1 (8%)	14,18,18	1.37	2 (14%)
1	GHP	O	4	1,3	10,11,12	0.82	0	11,14,16	1.01	0
1	OMZ	K	2[A]	1	12,14,15	1.52	2 (16%)	17,19,21	1.67	4 (23%)
1	3FG	C	7	1	12,13,13	1.22	2 (16%)	14,18,18	1.39	1 (7%)
1	GHP	M	4[A]	3	10,11,12	1.53	2 (20%)	11,14,16	1.43	2 (18%)
1	GHP	G	5	1	10,11,12	1.33	1 (10%)	11,14,16	1.15	1 (9%)
1	GHP	O	5	1	10,11,12	0.74	0	11,14,16	1.44	3 (27%)
1	MLU	C	1	1	7,8,9	1.18	1 (14%)	7,9,11	0.93	1 (14%)
1	GHP	K	4	1,3	10,11,12	1.38	1 (10%)	11,14,16	2.15	6 (54%)
1	OMY	I	6	1,4	12,14,15	0.98	1 (8%)	17,19,21	1.18	1 (5%)
1	OMZ	M	2	1	12,14,15	1.08	0	17,19,21	1.37	3 (17%)
1	GHP	M	5	1	10,11,12	0.89	0	11,14,16	1.31	1 (9%)
1	OMY	C	6	1,4	12,14,15	1.07	0	17,19,21	0.99	1 (5%)
1	MLU	K	1[A]	1	7,8,9	1.61	2 (28%)	7,9,11	1.60	2 (28%)
1	OMY	G	6[B]	4	12,14,15	1.17	1 (8%)	17,19,21	1.76	3 (17%)
1	OMY	K	6	1,4	12,14,15	1.09	1 (8%)	17,19,21	1.78	3 (17%)
1	3FG	E	7	1	12,13,13	1.01	1 (8%)	14,18,18	1.36	2 (14%)
1	OMY	O	6[B]	4	12,14,15	1.35	1 (8%)	17,19,21	1.79	3 (17%)
1	OMZ	O	2[B]	1	12,14,15	0.91	0	17,19,21	1.17	1 (5%)
1	MLU	E	1[B]	-	7,8,9	1.03	1 (14%)	7,9,11	1.13	1 (14%)
1	OMZ	I	2[B]	1	12,14,15	1.19	1 (8%)	17,19,21	1.04	1 (5%)
1	3FG	O	7	1	12,13,13	0.90	0	14,18,18	1.10	0
1	GHP	A	4	1,3	10,11,12	1.07	0	11,14,16	1.13	1 (9%)
1	3FG	I	7	1	12,13,13	1.31	2 (16%)	14,18,18	0.98	1 (7%)
1	OMY	M	6[B]	4	12,14,15	1.05	0	17,19,21	1.38	2 (11%)
1	GHP	A	5	1	10,11,12	1.29	1 (10%)	11,14,16	0.90	1 (9%)
1	3FG	M	7	1	12,13,13	1.38	3 (25%)	14,18,18	1.19	1 (7%)
1	MLU	O	1[B]	1	7,8,9	1.94	2 (28%)	7,9,11	2.28	2 (28%)
1	OMZ	G	2	1	12,14,15	1.14	1 (8%)	17,19,21	1.33	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLU	M	1	1	7,8,9	1.79	3 (42%)	7,9,11	2.07	1 (14%)
1	MLU	I	1[B]	1	7,8,9	1.70	1 (14%)	7,9,11	2.36	3 (42%)
1	OMY	A	6	1,4	12,14,15	1.31	1 (8%)	17,19,21	1.44	2 (11%)
1	OMY	O	6[A]	4	12,14,15	1.40	2 (16%)	17,19,21	1.67	4 (23%)
1	OMY	G	6[A]	4	12,14,15	1.18	1 (8%)	17,19,21	1.68	3 (17%)
1	OMZ	C	2	1	12,14,15	1.07	0	17,19,21	1.37	3 (17%)
1	OMZ	K	2[B]	1	12,14,15	1.51	2 (16%)	17,19,21	1.65	4 (23%)
1	OMZ	O	2[A]	1	12,14,15	0.90	0	17,19,21	1.27	2 (11%)
1	GHP	M	4[B]	3	10,11,12	1.53	2 (20%)	11,14,16	1.45	2 (18%)
1	MLU	E	1[A]	-	7,8,9	1.33	1 (14%)	7,9,11	1.52	1 (14%)
1	GHP	E	4	1,3	10,11,12	1.04	0	11,14,16	0.89	0
1	OMZ	I	2[A]	1	12,14,15	1.16	1 (8%)	17,19,21	1.01	1 (5%)
1	MLU	A	1	1	7,8,9	1.05	0	7,9,11	0.87	0
1	GHP	C	5	1	10,11,12	1.18	1 (10%)	11,14,16	1.04	0
1	MLU	G	1	1	7,8,9	0.64	0	7,9,11	1.39	1 (14%)
1	GHP	K	5	1	10,11,12	1.64	3 (30%)	11,14,16	1.82	2 (18%)
1	OMZ	A	2	1	12,14,15	1.05	1 (8%)	17,19,21	1.41	4 (23%)
1	OMY	M	6[A]	4	12,14,15	1.00	0	17,19,21	1.36	1 (5%)
1	GHP	G	4	1,3	10,11,12	1.05	0	11,14,16	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLU	K	1[B]	1	-	0/5/8/10	-
1	MLU	O	1[A]	1	-	2/5/8/10	-
1	GHP	I	4	1,3	-	0/4/6/8	0/1/1/1
1	3FG	G	7	1	-	2/8/8/8	0/1/1/1
1	GHP	E	5	1	-	0/4/6/8	0/1/1/1
1	MLU	I	1[A]	1	-	0/5/8/10	-
1	OMY	E	6	1,4	-	1/9/10/12	0/1/1/1
1	OMZ	E	2	1	-	0/9/10/12	0/1/1/1
1	GHP	C	4	1,3	-	1/4/6/8	0/1/1/1
1	GHP	I	5	1	-	0/4/6/8	0/1/1/1
1	3FG	K	7	1	-	2/8/8/8	0/1/1/1
1	3FG	A	7	1	-	2/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GHP	O	4	1,3	-	1/4/6/8	0/1/1/1
1	OMZ	K	2[A]	1	-	1/9/10/12	0/1/1/1
1	3FG	C	7	1	-	4/8/8/8	0/1/1/1
1	GHP	M	4[A]	3	-	1/4/6/8	0/1/1/1
1	GHP	G	5	1	-	0/4/6/8	0/1/1/1
1	GHP	O	5	1	-	0/4/6/8	0/1/1/1
1	MLU	C	1	1	-	0/5/8/10	-
1	GHP	K	4	1,3	-	0/4/6/8	0/1/1/1
1	OMY	I	6	1,4	-	1/9/10/12	0/1/1/1
1	OMZ	M	2	1	-	1/9/10/12	0/1/1/1
1	GHP	M	5	1	-	0/4/6/8	0/1/1/1
1	OMY	C	6	1,4	-	1/9/10/12	0/1/1/1
1	MLU	K	1[A]	1	-	0/5/8/10	-
1	OMY	G	6[B]	4	-	1/9/10/12	0/1/1/1
1	OMY	K	6	1,4	-	1/9/10/12	0/1/1/1
1	3FG	E	7	1	-	2/8/8/8	0/1/1/1
1	OMY	O	6[B]	4	-	1/9/10/12	0/1/1/1
1	OMZ	O	2[B]	1	-	1/9/10/12	0/1/1/1
1	MLU	E	1[B]	-	-	1/5/8/10	-
1	OMZ	I	2[B]	1	-	1/9/10/12	0/1/1/1
1	3FG	O	7	1	-	2/8/8/8	0/1/1/1
1	GHP	A	4	1,3	-	1/4/6/8	0/1/1/1
1	3FG	I	7	1	-	2/8/8/8	0/1/1/1
1	OMY	M	6[B]	4	-	1/9/10/12	0/1/1/1
1	GHP	A	5	1	-	0/4/6/8	0/1/1/1
1	3FG	M	7	1	-	2/8/8/8	0/1/1/1
1	MLU	O	1[B]	1	-	2/5/8/10	-
1	OMZ	G	2	1	-	0/9/10/12	0/1/1/1
1	MLU	M	1	1	-	2/5/8/10	-
1	MLU	I	1[B]	1	-	2/5/8/10	-
1	OMY	A	6	1,4	-	1/9/10/12	0/1/1/1
1	OMY	O	6[A]	4	-	1/9/10/12	0/1/1/1
1	OMY	G	6[A]	4	-	1/9/10/12	0/1/1/1
1	OMZ	C	2	1	-	0/9/10/12	0/1/1/1
1	OMZ	K	2[B]	1	-	1/9/10/12	0/1/1/1
1	OMZ	O	2[A]	1	-	1/9/10/12	0/1/1/1
1	GHP	M	4[B]	3	-	1/4/6/8	0/1/1/1
1	MLU	E	1[A]	-	-	0/5/8/10	-
1	GHP	E	4	1,3	-	0/4/6/8	0/1/1/1
1	OMZ	I	2[A]	1	-	1/9/10/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLU	A	1	1	-	0/5/8/10	-
1	GHP	C	5	1	-	0/4/6/8	0/1/1/1
1	MLU	G	1	1	-	1/5/8/10	-
1	GHP	K	5	1	-	0/4/6/8	0/1/1/1
1	OMZ	A	2	1	-	0/9/10/12	0/1/1/1
1	OMY	M	6[A]	4	-	1/9/10/12	0/1/1/1
1	GHP	G	4	1,3	-	1/4/6/8	0/1/1/1

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	1[B]	MLU	CB-CA	-3.99	1.48	1.53
1	M	4[A]	GHP	C1-CA	3.91	1.56	1.52
1	M	4[B]	GHP	C1-CA	3.91	1.56	1.52
1	K	1[A]	MLU	CB-CA	-3.60	1.49	1.53
1	I	1[B]	MLU	CA-N	3.55	1.53	1.47
1	K	2[A]	OMZ	CG-CB	-3.50	1.46	1.51
1	K	2[B]	OMZ	CG-CB	-3.50	1.46	1.51
1	O	1[A]	MLU	CB-CA	3.38	1.57	1.53
1	A	6	OMY	CD1-CG	3.35	1.44	1.39
1	A	5	GHP	CA-C	3.13	1.56	1.51
1	K	4	GHP	C3-C2	3.12	1.43	1.38
1	M	1	MLU	CN-N	3.01	1.54	1.46
1	O	1[A]	MLU	CA-N	2.94	1.52	1.47
1	E	1[A]	MLU	CN-N	2.90	1.54	1.46
1	C	4	GHP	C2-C1	-2.90	1.34	1.39
1	O	6[A]	OMY	CE2-CZ	-2.89	1.34	1.39
1	O	6[B]	OMY	CE2-CZ	-2.89	1.34	1.39
1	G	2	OMZ	CD1-CE1	-2.85	1.34	1.38
1	K	5	GHP	C6-C1	-2.78	1.34	1.39
1	M	1	MLU	CB-CA	-2.73	1.50	1.53
1	C	4	GHP	C1-CA	2.70	1.55	1.52
1	I	7	3FG	CZ-CD2	-2.65	1.35	1.39
1	G	5	GHP	C1-CA	2.62	1.55	1.52
1	K	6	OMY	OCZ-CZ	2.45	1.41	1.36
1	K	5	GHP	C3-C2	-2.43	1.34	1.38
1	M	7	3FG	CZ-CD2	-2.40	1.35	1.39
1	C	5	GHP	CA-C	2.40	1.55	1.51
1	O	1[B]	MLU	CA-N	2.34	1.51	1.47
1	K	5	GHP	CA-C	2.33	1.54	1.51
1	I	4	GHP	C3-C2	2.33	1.42	1.38
1	I	5	GHP	C3-C2	-2.33	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	4	GHP	C6-C5	2.32	1.42	1.38
1	C	7	3FG	CG1-CD1	2.28	1.42	1.39
1	I	4	GHP	C6-C1	-2.26	1.35	1.39
1	I	7	3FG	OXT-C	-2.26	1.23	1.30
1	M	4[A]	GHP	C2-C1	-2.25	1.35	1.39
1	M	4[B]	GHP	C2-C1	-2.25	1.35	1.39
1	A	2	OMZ	OH-CZ	2.24	1.40	1.36
1	O	1[A]	MLU	CN-N	2.23	1.52	1.46
1	I	2[B]	OMZ	CA-N	-2.22	1.41	1.47
1	C	1	MLU	CB-CA	-2.18	1.51	1.53
1	M	1	MLU	CA-N	2.18	1.51	1.47
1	K	2[A]	OMZ	OH-CZ	2.17	1.40	1.36
1	K	2[B]	OMZ	OH-CZ	2.17	1.40	1.36
1	E	2	OMZ	CD1-CE1	-2.17	1.35	1.38
1	C	7	3FG	OXT-C	-2.15	1.23	1.30
1	K	7	3FG	CG2-CB	2.14	1.42	1.39
1	E	1[B]	MLU	CN-N	2.12	1.52	1.46
1	E	7	3FG	CG1-CD1	2.11	1.42	1.39
1	K	1[A]	MLU	CN-N	2.11	1.52	1.46
1	C	4	GHP	C3-C2	2.10	1.42	1.38
1	G	6[A]	OMY	CE2-CZ	-2.09	1.35	1.39
1	G	6[B]	OMY	CE2-CZ	-2.09	1.35	1.39
1	K	1[B]	MLU	CN-N	2.06	1.51	1.46
1	O	6[A]	OMY	CG-CB	-2.06	1.48	1.51
1	M	7	3FG	OXT-C	-2.05	1.24	1.30
1	A	7	3FG	CZ-CD2	-2.04	1.36	1.39
1	I	6	OMY	OCZ-CZ	2.03	1.40	1.36
1	I	2[A]	OMZ	CA-N	-2.02	1.41	1.47
1	M	7	3FG	CG1-CB	2.01	1.42	1.39

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	1[B]	MLU	CB-CA-N	-4.91	103.15	110.59
1	M	6[A]	OMY	CG-CB-CA	-4.66	105.46	111.58
1	G	6[A]	OMY	CD1-CE1-CZ	-4.52	118.29	120.92
1	G	6[B]	OMY	CD1-CE1-CZ	-4.52	118.29	120.92
1	M	1	MLU	CB-CA-N	4.45	117.34	110.59
1	M	6[B]	OMY	CG-CB-CA	-4.45	105.74	111.58
1	O	6[B]	OMY	CG-CB-CA	-4.15	106.12	111.58
1	K	6	OMY	CE2-CZ-CE1	4.11	122.36	118.49
1	K	6	OMY	CD1-CE1-CZ	-4.05	118.56	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	1[B]	MLU	CD1-CG-CB	4.03	125.59	111.08
1	O	6[A]	OMY	CD1-CE1-CZ	-4.03	118.57	120.92
1	O	6[B]	OMY	CD1-CE1-CZ	-4.03	118.57	120.92
1	G	6[B]	OMY	CG-CB-CA	-3.88	106.49	111.58
1	K	5	GHP	C6-C5-C4	-3.87	115.78	119.88
1	O	1[B]	MLU	CB-CA-C	3.85	116.92	110.99
1	K	4	GHP	C3-C2-C1	-3.65	117.54	121.18
1	C	7	3FG	CD1-CG1-CB	-3.53	117.04	120.09
1	K	2[A]	OMZ	CD2-CG-CB	3.52	126.01	120.71
1	K	2[B]	OMZ	CD2-CG-CB	3.52	126.01	120.71
1	A	6	OMY	CG-CB-CA	-3.42	107.09	111.58
1	I	1[A]	MLU	CB-CA-N	-3.41	105.42	110.59
1	G	2	OMZ	CD2-CE2-CZ	-3.35	117.15	120.50
1	K	4	GHP	C6-C5-C4	3.27	123.34	119.88
1	C	2	OMZ	CD1-CE1-CZ	-3.21	119.05	120.92
1	O	6[A]	OMY	CG-CB-CA	-3.21	107.36	111.58
1	O	1[A]	MLU	CD2-CG-CD1	-3.20	96.25	110.53
1	G	1	MLU	CB-CA-C	-3.20	106.07	110.99
1	G	6[A]	OMY	CG-CB-CA	-3.19	107.39	111.58
1	K	1[A]	MLU	CB-CA-C	3.16	115.85	110.99
1	K	5	GHP	C5-C6-C1	3.09	124.27	121.18
1	E	1[A]	MLU	CB-CA-C	-3.08	106.25	110.99
1	E	5	GHP	C6-C5-C4	-3.06	116.64	119.88
1	K	4	GHP	C2-C3-C4	3.06	123.12	119.88
1	A	7	3FG	CD1-CG1-CB	-3.06	117.45	120.09
1	E	7	3FG	CD1-CG1-CB	-3.05	117.45	120.09
1	K	1[B]	MLU	CB-CA-N	-2.88	106.23	110.59
1	M	2	OMZ	O-C-CA	-2.77	117.64	124.77
1	E	2	OMZ	O-C-CA	-2.76	117.66	124.77
1	E	6	OMY	CG-CB-CA	-2.74	107.98	111.58
1	O	2[A]	OMZ	O-C-CA	-2.71	117.81	124.77
1	O	2[A]	OMZ	CD1-CE1-CZ	-2.67	119.36	120.92
1	O	2[B]	OMZ	CD1-CE1-CZ	-2.67	119.36	120.92
1	O	6[A]	OMY	CE2-CZ-CE1	2.66	120.99	118.49
1	O	6[B]	OMY	CE2-CZ-CE1	2.66	120.99	118.49
1	E	6	OMY	CD1-CE1-CZ	-2.61	119.40	120.92
1	E	1[B]	MLU	CB-CA-C	-2.61	106.98	110.99
1	K	7	3FG	CD1-CG1-CB	-2.61	117.84	120.09
1	O	5	GHP	C6-C5-C4	-2.55	117.18	119.88
1	A	2	OMZ	CE2-CZ-CE1	2.54	120.88	118.49
1	K	6	OMY	CG-CB-CA	-2.53	108.25	111.58
1	M	5	GHP	C1-CA-C	-2.52	105.01	112.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	7	3FG	CG2-CB-CG1	2.52	121.53	118.09
1	K	1[B]	MLU	CD2-CG-CB	2.51	120.10	111.08
1	C	6	OMY	CG-CB-CA	-2.50	108.30	111.58
1	M	2	OMZ	CD2-CE2-CZ	-2.50	118.00	120.50
1	A	2	OMZ	CD1-CE1-CZ	-2.48	119.48	120.92
1	G	5	GHP	C1-CA-C	-2.47	105.15	112.09
1	K	2[A]	OMZ	CD2-CE2-CZ	-2.47	118.03	120.50
1	K	2[B]	OMZ	CD2-CE2-CZ	-2.47	118.03	120.50
1	A	7	3FG	CG2-CB-CG1	2.46	121.45	118.09
1	K	7	3FG	CD2-CG2-CB	-2.44	117.98	120.09
1	I	4	GHP	C6-C1-C2	2.43	121.32	118.30
1	K	4	GHP	C5-C6-C1	-2.43	118.76	121.18
1	I	5	GHP	C1-CA-C	-2.39	105.37	112.09
1	A	2	OMZ	O-C-CA	-2.39	118.62	124.77
1	C	2	OMZ	O-C-CA	-2.39	118.63	124.77
1	G	2	OMZ	O-C-CA	-2.37	118.67	124.77
1	G	6[A]	OMY	CE2-CZ-CE1	2.34	120.69	118.49
1	G	6[B]	OMY	CE2-CZ-CE1	2.34	120.69	118.49
1	I	6	OMY	CE2-CZ-CE1	2.33	120.68	118.49
1	C	1	MLU	O-C-CA	-2.31	118.83	124.77
1	I	1[B]	MLU	CN-N-CA	-2.31	106.80	113.70
1	M	7	3FG	CD2-CG2-CB	-2.31	118.10	120.09
1	G	2	OMZ	CE2-CZ-CE1	2.29	120.64	118.49
1	M	4[A]	GHP	C3-C2-C1	-2.29	118.90	121.18
1	M	4[B]	GHP	C3-C2-C1	-2.29	118.90	121.18
1	M	2	OMZ	CE2-CZ-CE1	2.29	120.64	118.49
1	G	7	3FG	CD1-CG1-CB	-2.27	118.13	120.09
1	C	4	GHP	C5-C6-C1	-2.26	118.92	121.18
1	A	6	OMY	CD1-CE1-CZ	2.26	122.25	120.92
1	K	2[A]	OMZ	CD1-CG-CB	-2.26	115.75	119.55
1	K	2[B]	OMZ	CD1-CG-CB	-2.26	115.75	119.55
1	C	2	OMZ	CE2-CZ-CE1	2.24	120.60	118.49
1	K	7	3FG	CZ-CD1-CG1	2.21	123.51	120.47
1	K	2[A]	OMZ	CE2-CD2-CG	2.21	123.39	121.18
1	K	2[B]	OMZ	CE2-CD2-CG	2.21	123.39	121.18
1	I	2[B]	OMZ	O-C-CA	-2.16	119.22	124.77
1	E	2	OMZ	CD1-CE1-CL	2.16	121.98	118.45
1	A	4	GHP	C5-C6-C1	-2.15	119.04	121.18
1	K	1[A]	MLU	CD2-CG-CD1	-2.15	100.94	110.53
1	M	6[B]	OMY	ODE-CB-CA	-2.15	102.77	107.49
1	K	4	GHP	C5-C4-C3	-2.14	116.35	119.77
1	K	1[B]	MLU	O-C-CA	-2.14	119.26	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	1[B]	MLU	CB-CA-C	2.13	114.27	110.99
1	I	7	3FG	CD1-CG1-CB	-2.12	118.26	120.09
1	M	4[A]	GHP	C2-C3-C4	2.10	122.10	119.88
1	M	4[B]	GHP	C2-C3-C4	2.10	122.10	119.88
1	E	5	GHP	C5-C6-C1	2.10	123.28	121.18
1	O	6[A]	OMY	CD2-CG-CB	2.07	123.83	120.71
1	A	2	OMZ	CD2-CE2-CZ	-2.07	118.43	120.50
1	C	4	GHP	C6-C5-C4	2.06	122.06	119.88
1	O	5	GHP	C2-C3-C4	2.04	122.04	119.88
1	O	5	GHP	C1-CA-C	-2.03	106.40	112.09
1	K	4	GHP	C6-C1-C2	2.02	120.81	118.30
1	A	5	GHP	C1-CA-C	-2.01	106.46	112.09
1	I	2[A]	OMZ	O-C-CA	-2.00	119.62	124.77

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	6	OMY	O-C-CA-CB
1	C	6	OMY	O-C-CA-CB
1	E	6	OMY	O-C-CA-CB
1	G	6[A]	OMY	O-C-CA-CB
1	G	6[B]	OMY	O-C-CA-CB
1	I	6	OMY	O-C-CA-CB
1	K	6	OMY	O-C-CA-CB
1	M	6[A]	OMY	O-C-CA-CB
1	M	6[B]	OMY	O-C-CA-CB
1	O	6[A]	OMY	O-C-CA-CB
1	O	6[B]	OMY	O-C-CA-CB
1	E	1[B]	MLU	O-C-CA-CB
1	G	1	MLU	O-C-CA-CB
1	O	1[A]	MLU	C-CA-CB-CG
1	K	2[A]	OMZ	O-C-CA-CB
1	K	2[B]	OMZ	O-C-CA-CB
1	M	2	OMZ	O-C-CA-CB
1	O	2[A]	OMZ	O-C-CA-CB
1	A	7	3FG	C-CA-CB-CG1
1	C	7	3FG	C-CA-CB-CG1
1	C	7	3FG	C-CA-CB-CG2
1	E	7	3FG	C-CA-CB-CG1
1	E	7	3FG	C-CA-CB-CG2
1	I	1[B]	MLU	CA-CB-CG-CD2

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Mol	Chain	Res	Type	Atoms
1	O	1[A]	MLU	N-CA-CB-CG
1	O	1[B]	MLU	CA-CB-CG-CD2
1	I	1[B]	MLU	CA-CB-CG-CD1
1	O	1[B]	MLU	CA-CB-CG-CD1
1	A	7	3FG	C-CA-CB-CG2
1	G	7	3FG	C-CA-CB-CG1
1	G	7	3FG	C-CA-CB-CG2
1	M	1	MLU	N-CA-CB-CG
1	I	7	3FG	C-CA-CB-CG1
1	I	7	3FG	C-CA-CB-CG2
1	K	7	3FG	C-CA-CB-CG2
1	M	7	3FG	C-CA-CB-CG2
1	O	7	3FG	C-CA-CB-CG1
1	O	7	3FG	C-CA-CB-CG2
1	M	1	MLU	C-CA-CB-CG
1	K	7	3FG	C-CA-CB-CG1
1	C	7	3FG	O-C-CA-CB
1	C	7	3FG	OXT-C-CA-CB
1	M	7	3FG	C-CA-CB-CG1
1	A	4	GHP	C2-C1-CA-C
1	C	4	GHP	C2-C1-CA-C
1	G	4	GHP	C6-C1-CA-N
1	M	4[A]	GHP	C6-C1-CA-N
1	M	4[B]	GHP	C6-C1-CA-N
1	O	4	GHP	C6-C1-CA-N
1	I	2[A]	OMZ	O-C-CA-CB
1	I	2[B]	OMZ	O-C-CA-CB
1	O	2[B]	OMZ	O-C-CA-CB

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	1[A]	MLU	2	0
1	C	1	MLU	1	0
1	I	6	OMY	1	0
1	K	1[A]	MLU	1	0
1	O	1[B]	MLU	1	0
1	M	1	MLU	1	0
1	G	6[A]	OMY	1	0
1	C	2	OMZ	1	0
1	A	2	OMZ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

28 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CIT	E	20	-	8,8,12	1.66	2 (25%)	10,10,17	2.86	3 (30%)
6	MRD	I	21	-	7,7,7	0.78	0	9,10,10	0.93	0
4	DVC	I	9	1	10,11,12	2.54	2 (20%)	9,18,20	1.13	1 (11%)
3	BGC	M	8[B]	1	11,11,12	2.44	6 (54%)	15,15,17	1.24	1 (6%)
4	DVC	G	9[B]	1	10,11,12	4.70	4 (40%)	9,18,20	2.08	3 (33%)
4	DVC	K	9	1	10,11,12	3.09	2 (20%)	9,18,20	1.37	2 (22%)
3	BGC	G	8	1	11,11,12	1.71	3 (27%)	15,15,17	0.98	0
4	DVC	O	9[A]	1	10,11,12	2.83	2 (20%)	9,18,20	2.05	1 (11%)
3	BGC	O	8[B]	-	11,11,12	2.07	2 (18%)	15,15,17	1.19	3 (20%)
3	BGC	I	8	1	11,11,12	1.85	3 (27%)	15,15,17	1.14	1 (6%)
4	DVC	M	9[B]	1	10,11,12	4.49	3 (30%)	9,18,20	2.13	4 (44%)
5	CIT	O	20	-	12,12,12	1.79	3 (25%)	17,17,17	1.87	5 (29%)
5	CIT	M	20	-	12,12,12	1.71	3 (25%)	17,17,17	1.96	6 (35%)
4	DVC	A	9	1	10,11,12	1.64	2 (20%)	9,18,20	1.71	1 (11%)
4	DVC	G	9[A]	1	10,11,12	4.72	3 (30%)	9,18,20	2.41	2 (22%)
5	CIT	K	20	-	5,5,12	0.92	0	5,5,17	1.67	2 (40%)
3	BGC	K	8	1	11,11,12	2.15	4 (36%)	15,15,17	1.34	1 (6%)
3	BGC	M	8[A]	1	11,11,12	2.61	6 (54%)	15,15,17	1.51	3 (20%)
7	MPD	K	21	-	7,7,7	1.12	1 (14%)	9,10,10	0.92	1 (11%)
3	BGC	A	8	1	11,11,12	1.31	1 (9%)	15,15,17	0.58	0
4	DVC	C	9	1	10,11,12	2.74	4 (40%)	9,18,20	1.84	2 (22%)
3	BGC	O	8[A]	-	11,11,12	1.97	2 (18%)	15,15,17	1.27	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	E	8	1	11,11,12	1.93	3 (27%)	15,15,17	0.85	0
4	DVC	M	9[A]	1	10,11,12	3.89	3 (30%)	9,18,20	1.20	1 (11%)
5	CIT	I	20	-	12,12,12	1.86	4 (33%)	17,17,17	3.24	7 (41%)
4	DVC	E	9	1	10,11,12	3.30	3 (30%)	9,18,20	1.80	2 (22%)
4	DVC	O	9[B]	1	10,11,12	4.21	3 (30%)	9,18,20	1.44	2 (22%)
3	BGC	C	8	1	11,11,12	1.24	1 (9%)	15,15,17	0.99	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DVC	O	9[B]	1	-	-	0/1/1/1
4	DVC	I	9	1	-	-	0/1/1/1
3	BGC	M	8[B]	1	-	0/2/19/22	0/1/1/1
4	DVC	G	9[B]	1	-	-	0/1/1/1
4	DVC	K	9	1	-	-	0/1/1/1
3	BGC	G	8	1	-	0/2/19/22	0/1/1/1
4	DVC	O	9[A]	1	-	-	0/1/1/1
3	BGC	O	8[B]	-	-	0/2/19/22	0/1/1/1
3	BGC	I	8	1	-	0/2/19/22	0/1/1/1
4	DVC	M	9[B]	1	-	-	0/1/1/1
5	CIT	O	20	-	-	2/16/16/16	-
5	CIT	M	20	-	-	4/16/16/16	-
4	DVC	A	9	1	-	-	0/1/1/1
3	BGC	C	8	1	-	0/2/19/22	0/1/1/1
4	DVC	G	9[A]	1	-	-	0/1/1/1
5	CIT	K	20	-	-	2/3/3/16	-
3	BGC	K	8	1	-	0/2/19/22	0/1/1/1
3	BGC	M	8[A]	1	-	0/2/19/22	0/1/1/1
7	MPD	K	21	-	-	0/5/5/5	-
3	BGC	A	8	1	-	0/2/19/22	0/1/1/1
4	DVC	C	9	1	-	-	0/1/1/1
3	BGC	O	8[A]	-	-	1/2/19/22	0/1/1/1
3	BGC	E	8	1	-	0/2/19/22	0/1/1/1
5	CIT	I	20	-	-	7/16/16/16	-
4	DVC	M	9[A]	1	-	-	0/1/1/1
4	DVC	E	9	1	-	-	0/1/1/1
6	MRD	I	21	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CIT	E	20	-	-	1/8/8/16	-

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	9[A]	DVC	O4-C4	12.19	1.52	1.40
4	G	9[B]	DVC	O4-C4	11.51	1.51	1.40
4	M	9[B]	DVC	O4-C4	10.95	1.50	1.40
4	O	9[B]	DVC	O4-C4	10.34	1.50	1.40
4	M	9[A]	DVC	O4-C4	9.47	1.49	1.40
4	O	9[A]	DVC	O4-C4	8.09	1.48	1.40
4	K	9	DVC	O4-C4	7.50	1.47	1.40
4	O	9[B]	DVC	O41-C4	7.47	1.47	1.40
4	M	9[A]	DVC	O41-C4	6.93	1.46	1.40
4	E	9	DVC	O41-C4	6.88	1.46	1.40
4	C	9	DVC	O4-C4	6.84	1.46	1.40
4	E	9	DVC	O4-C4	6.41	1.46	1.40
4	I	9	DVC	O4-C4	6.30	1.46	1.40
4	G	9[B]	DVC	C4-C5	6.28	1.59	1.53
4	G	9[A]	DVC	C4-C5	6.10	1.59	1.53
4	G	9[B]	DVC	O41-C4	6.10	1.46	1.40
4	M	9[B]	DVC	O41-C4	6.10	1.46	1.40
4	K	9	DVC	C4-C5	5.97	1.59	1.53
4	M	9[B]	DVC	C4-C5	5.87	1.59	1.53
4	G	9[A]	DVC	O41-C4	5.11	1.45	1.40
3	M	8[B]	BGC	C2-C3	-5.10	1.44	1.52
3	M	8[A]	BGC	O5-C5	5.08	1.53	1.43
3	O	8[A]	BGC	O5-C1	-4.71	1.35	1.43
3	O	8[B]	BGC	O5-C1	-4.71	1.35	1.43
4	I	9	DVC	C4-C5	4.24	1.57	1.53
3	E	8	BGC	O5-C1	-4.22	1.36	1.43
4	E	9	DVC	C4-C5	3.92	1.57	1.53
3	K	8	BGC	C4-C5	-3.71	1.45	1.53
5	I	20	CIT	C4-C3	-3.67	1.49	1.54
3	K	8	BGC	C2-C3	-3.67	1.46	1.52
3	M	8[B]	BGC	O5-C5	3.66	1.50	1.43
3	O	8[B]	BGC	O5-C5	3.60	1.50	1.43
3	M	8[A]	BGC	C2-C3	-3.53	1.47	1.52
4	A	9	DVC	C4-C5	3.38	1.56	1.53
3	M	8[A]	BGC	C4-C5	-3.29	1.46	1.53
5	M	20	CIT	C3-C6	-3.24	1.50	1.53
5	O	20	CIT	O7-C3	-3.21	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	8	BGC	C6-C5	3.20	1.62	1.51
3	I	8	BGC	C4-C5	-3.19	1.46	1.53
3	M	8[A]	BGC	O5-C1	-3.15	1.38	1.43
3	G	8	BGC	C6-C5	3.14	1.62	1.51
3	A	8	BGC	O5-C1	-3.11	1.38	1.43
5	I	20	CIT	O7-C3	3.10	1.49	1.43
3	I	8	BGC	C2-C3	-2.96	1.48	1.52
3	E	8	BGC	C2-C3	-2.95	1.48	1.52
3	E	8	BGC	C6-C5	2.94	1.61	1.51
5	M	20	CIT	O7-C3	-2.91	1.37	1.43
3	I	8	BGC	C6-C5	2.79	1.61	1.51
5	E	20	CIT	O7-C3	-2.79	1.36	1.42
4	O	9[A]	DVC	O41-C4	2.78	1.42	1.40
3	O	8[A]	BGC	O5-C5	2.77	1.48	1.43
4	C	9	DVC	O41-C4	2.77	1.42	1.40
5	M	20	CIT	O4-C5	-2.76	1.21	1.30
3	K	8	BGC	O5-C5	2.71	1.48	1.43
4	C	9	DVC	C2-C3	-2.71	1.50	1.54
3	M	8[B]	BGC	C6-C5	2.70	1.60	1.51
3	G	8	BGC	O5-C1	-2.55	1.39	1.43
3	M	8[A]	BGC	O6-C6	-2.54	1.31	1.42
5	E	20	CIT	O5-C6	2.50	1.29	1.22
3	M	8[B]	BGC	O5-C1	-2.49	1.39	1.43
4	O	9[B]	DVC	C4-C5	2.44	1.55	1.53
5	O	20	CIT	O4-C5	-2.33	1.23	1.30
4	A	9	DVC	O4-C4	2.33	1.42	1.40
4	M	9[A]	DVC	C4-C5	2.29	1.55	1.53
3	G	8	BGC	O5-C5	2.28	1.47	1.43
5	O	20	CIT	O2-C1	-2.22	1.23	1.30
3	M	8[B]	BGC	O6-C6	-2.22	1.33	1.42
4	G	9[B]	DVC	C2-C3	-2.21	1.51	1.54
5	I	20	CIT	O1-C1	2.16	1.29	1.22
3	C	8	BGC	O5-C1	-2.15	1.40	1.43
4	C	9	DVC	C3-C4	-2.13	1.49	1.53
7	K	21	MPD	CM-C2	-2.10	1.46	1.52
3	M	8[B]	BGC	C4-C5	-2.04	1.48	1.53
3	M	8[A]	BGC	C6-C5	2.03	1.58	1.51
5	I	20	CIT	O4-C5	-2.00	1.24	1.30

All (57) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	20	CIT	O7-C3-C6	-9.62	95.31	108.96
5	E	20	CIT	O7-C3-C2	7.98	129.18	109.96
4	O	9[A]	DVC	C1-O5-C5	5.59	117.70	111.53
4	G	9[A]	DVC	O5-C1-C2	5.41	118.72	111.38
5	O	20	CIT	O7-C3-C6	-5.36	101.36	108.96
4	M	9[B]	DVC	C1-O5-C5	4.75	116.77	111.53
4	G	9[B]	DVC	C1-O5-C5	4.66	116.67	111.53
5	I	20	CIT	O5-C6-C3	-4.66	113.07	122.09
4	A	9	DVC	C1-O5-C5	4.51	116.51	111.53
4	C	9	DVC	C1-O5-C5	4.41	116.40	111.53
3	K	8	BGC	C1-O5-C5	-3.94	106.90	112.19
4	E	9	DVC	C1-O5-C5	3.93	115.87	111.53
5	M	20	CIT	O3-C5-C4	-3.77	112.26	122.95
5	I	20	CIT	O6-C6-O5	3.60	135.37	123.86
4	O	9[B]	DVC	C1-O5-C5	3.35	115.23	111.53
3	O	8[A]	BGC	O5-C5-C6	-3.34	101.16	107.66
5	I	20	CIT	O2-C1-C2	3.33	124.88	114.35
3	M	8[A]	BGC	C1-O5-C5	-3.25	107.83	112.19
4	G	9[A]	DVC	O4-C4-C5	-3.19	102.76	110.53
5	I	20	CIT	C2-C3-C6	3.10	116.88	110.03
4	K	9	DVC	C1-O5-C5	3.05	114.89	111.53
5	I	20	CIT	O4-C5-O3	-3.04	115.52	123.33
5	M	20	CIT	O1-C1-C2	-2.99	114.48	122.95
5	M	20	CIT	O4-C5-C4	2.96	123.73	114.35
4	M	9[A]	DVC	C1-O5-C5	2.91	114.74	111.53
3	O	8[B]	BGC	C1-O5-C5	-2.69	108.58	112.19
5	M	20	CIT	C4-C3-C6	2.67	115.95	110.03
5	I	20	CIT	O1-C1-C2	-2.63	115.50	122.95
5	K	20	CIT	C3-C2-C1	2.56	116.62	113.11
4	G	9[B]	DVC	C2-C3-N3	2.52	111.79	107.56
4	M	9[B]	DVC	O4-C4-C3	-2.51	103.03	108.92
4	M	9[B]	DVC	O41-C4-C5	-2.51	104.41	110.53
5	O	20	CIT	O1-C1-C2	-2.50	115.86	122.95
5	O	20	CIT	O7-C3-C2	2.49	115.05	109.38
4	C	9	DVC	O41-C4-C3	2.45	114.65	108.92
5	E	20	CIT	O2-C1-C2	-2.41	106.52	114.00
5	E	20	CIT	C2-C3-C6	-2.38	104.69	110.53
4	I	9	DVC	C1-O5-C5	2.36	114.14	111.53
3	I	8	BGC	C1-O5-C5	-2.32	109.08	112.19
3	M	8[A]	BGC	O5-C5-C6	-2.27	103.24	107.66
3	M	8[A]	BGC	C1-C2-C3	-2.25	106.36	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	9[B]	DVC	O4-C4-C5	-2.24	105.08	110.53
4	E	9	DVC	O5-C1-C2	-2.22	108.37	111.38
3	C	8	BGC	O5-C5-C6	-2.20	103.38	107.66
3	O	8[B]	BGC	O5-C5-C6	-2.16	103.46	107.66
5	K	20	CIT	O7-C3-C2	2.13	118.95	110.96
4	O	9[B]	DVC	O5-C1-C2	2.12	114.25	111.38
5	O	20	CIT	O2-C1-C2	2.09	120.96	114.35
4	M	9[B]	DVC	O41-C4-C3	2.08	113.80	108.92
3	O	8[B]	BGC	O5-C5-C4	-2.07	105.79	110.83
5	M	20	CIT	C3-C4-C5	-2.06	108.29	113.92
5	O	20	CIT	C3-C4-C5	2.05	119.54	113.92
7	K	21	MPD	O2-C2-CM	-2.03	101.66	107.99
3	O	8[A]	BGC	C1-O5-C5	-2.03	109.47	112.19
4	K	9	DVC	C2-C3-C4	2.03	109.17	107.12
5	M	20	CIT	O6-C6-C3	2.00	116.98	113.14
3	M	8[B]	BGC	C1-O5-C5	-2.00	109.50	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	20	CIT	C1-C2-C3-O7
5	I	20	CIT	C1-C2-C3-O7
5	I	20	CIT	C1-C2-C3-C4
5	I	20	CIT	C1-C2-C3-C6
3	O	8[A]	BGC	O5-C5-C6-O6
5	M	20	CIT	O1-C1-C2-C3
5	M	20	CIT	O2-C1-C2-C3
5	I	20	CIT	C2-C3-C6-O6
5	E	20	CIT	O2-C1-C2-C3
5	I	20	CIT	C2-C3-C6-O5
5	O	20	CIT	O1-C1-C2-C3
5	I	20	CIT	O2-C1-C2-C3
5	O	20	CIT	O2-C1-C2-C3
5	I	20	CIT	O1-C1-C2-C3
5	M	20	CIT	C3-C4-C5-O4
5	K	20	CIT	O2-C1-C2-C3
5	M	20	CIT	C3-C4-C5-O3

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	20	CIT	3	0
4	G	9[B]	DVC	3	0
4	O	9[A]	DVC	1	0
4	G	9[A]	DVC	1	0
5	K	20	CIT	1	0
5	I	20	CIT	2	0
4	E	9	DVC	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.